



## The influence of molecular structure of fatty acid monoalkyl esters on diesel combustion

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### ABSTRACT

The subject of this paper is a series of experiments conducted on a single-cylinder research engine investigating the influence of molecular structure on the combustion behaviour of fatty acid alcohol ester (biodiesel) molecules under diesel engine conditions. The fuels employed in these experiments comprised various samples of pure individual fatty acid alcohol ester molecules of different structure, as well as several mixtures of such molecules. The latter consisted in biodiesel fuels produced by the transesterification of naturally occurring plant oils or animal fat with a monohydric alcohol. It was observed that the molecular structure of the fuel significantly influenced the formation of NO<sub>x</sub> and particulate matter and their respective concentration in the exhaust gas. The influence on the formation of NO<sub>x</sub> in particular, appeared to be exerted first through the effect which the molecular structure had on the auto-ignition delay occurring after the fuel was injected into the combustion chamber, and second through the flame temperature at which the various molecules burned. The emission of particulates on the other hand showed correlation with the number of double bonds in the fuel molecules for the case of larger accumulation mode particles, and with the boiling point of the fuel samples for the case of the smaller, nucleation mode particles. The effect of ignition delay on the exhaust emissions of these pollutants was isolated by adding the ignition promoting molecule 2-ethylhexyl nitrate to some of the fuel samples in closely specified concentrations, so as to equalise the ignition delay for the relevant fuel samples. The removal of the ignition delay as a main influence on the combustion process enabled the observation of the lesser effects of adiabatic flame temperature.

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### 1. Introduction

The combustion of biomass-derived liquid fuels such as biodiesel has gained significant importance in practical combustion systems such as diesel engines. An understanding of the physical and chemical processes occurring during their combustion, especially those which significantly influence the thermal efficiency and the formation of pollutants is important, not least, for the development of better alternatives.

Biodiesel is defined as a liquid hydrocarbon fuel composed of fatty acid monohydric alcohol esters whose molecular composition may change according to the feed-stocks used for the fuel synthesis [1]. Differences in molecular structure influence the physical and chemical processes occurring during the atomisation, vaporisation and combustion of the fuel after it is injected into the combustion chamber. These differences lead to distinctive patterns in

fuel energy release rates and pollutant formation from various molecules.

Several researchers have reported that the combustion of biodiesel in diesel engines tends to result in lower emissions of particulate mass (PM), unburned hydrocarbons (UHC) and carbon monoxide (CO) with respect to fossil diesel fuel, along with a small increase in the emission of nitrogen oxides (NO<sub>x</sub>) [2–10]. The reasons for these changes are still not fully understood, and are expected to depend in detail on the mixture of chemical species present in the biodiesel fuel.

It is generally accepted that the low particulate mass emission from biodiesel is a result of the fuel-bound oxygen, which lowers the oxygen equivalence ratio ( $\Phi_{O_2}$ ) of combustion in the fuel-rich zones of the fuel spray, and aids the oxidation of soot and its precursors. An optical study of biodiesel flames has shown that  $\Phi_{O_2}$  at the lift-off length of biodiesel-fuelled diesel engine flames is significantly lower than for a primary reference fuel representative of fossil diesel fuel, if the fuel-bound oxygen of biodiesel is taken into account [11]. This could provide a plausible explanation for the lower rate of formation of soot and its precursors within the fuel-rich premixed flames of the combustion process. The

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